Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 07:46 AM EST

PDB ID	:	3PJW
Title	:	Structure of Pseudomonas fluorescence LapD GGDEF-EAL dual domain, I23
Authors	:	Sondermann, H.; Navarro, M.V.A.S.
Deposited on	:	2010-11-10
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

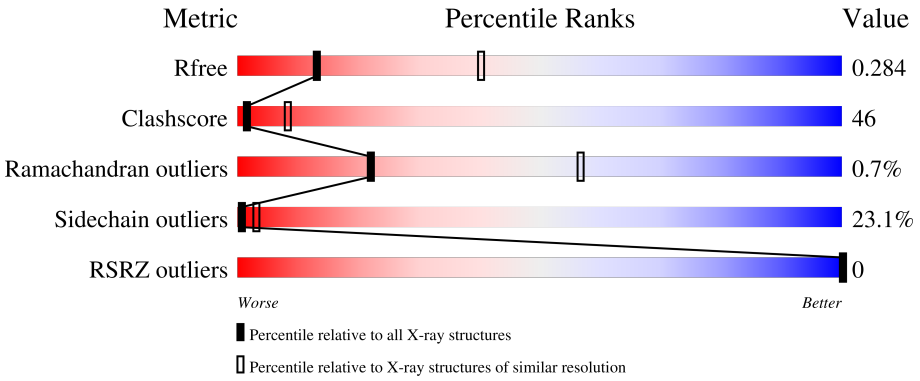
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	40% 44% 13% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3315 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyclic dimeric GMP binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	423	3315	2078	600	629	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

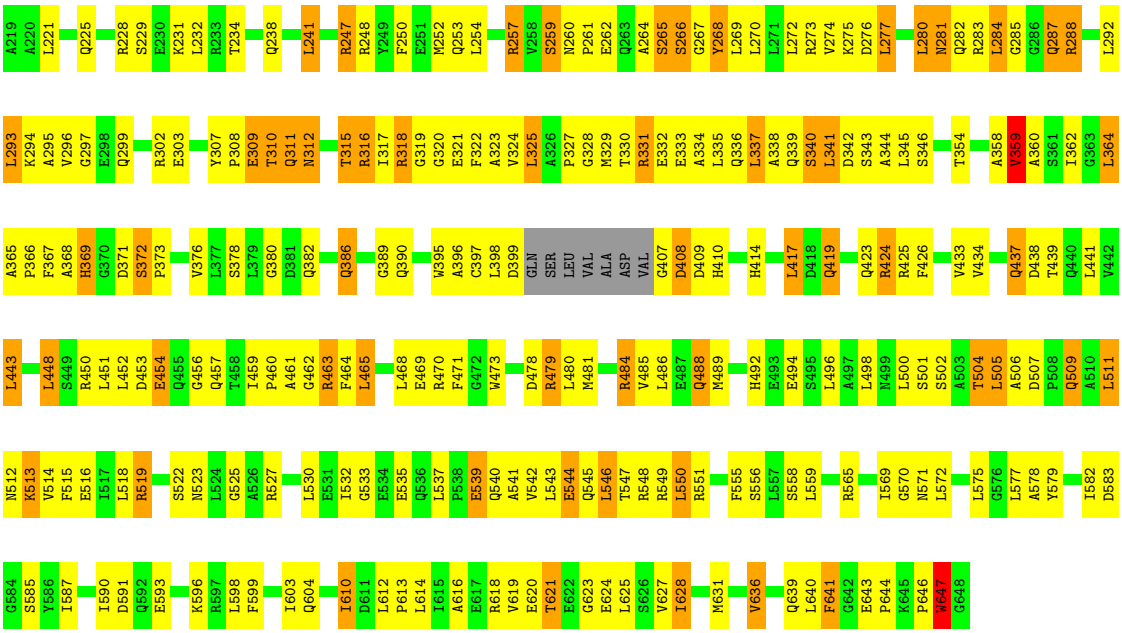
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	-	expression tag	UNP Q3KK31

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cyclic dimeric GMP binding protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	154.84Å 154.84Å 154.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 3.10 48.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.97-3.10) 98.9 (48.97-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.234 , 0.284 0.232 , 0.284	Depositor DCC
R_{free} test set	539 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	87.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.017 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3315	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.53	0/3368	0.69	0/4550

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3315	0	3299	302	0
All	All	3315	0	3299	302	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HD12	1:A:337:LEU:O	1.35	1.20
1:A:307:TYR:O	1:A:310:THR:HG23	1.41	1.18
1:A:330:THR:OG1	1:A:333:GLU:CG	1.92	1.18
1:A:514:VAL:O	1:A:518:LEU:HD12	1.48	1.14
1:A:264:ALA:HB1	1:A:265:SER:HB2	1.17	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:HG1	1:A:333:GLU:HG3	1.15	1.12
1:A:330:THR:OG1	1:A:333:GLU:HG3	1.49	1.09
1:A:341:LEU:HD12	1:A:341:LEU:O	1.51	1.09
1:A:316:ARG:HB2	1:A:322:PHE:CD1	1.88	1.06
1:A:417:LEU:HD22	1:A:468:LEU:HD21	1.34	1.04
1:A:264:ALA:HB1	1:A:265:SER:CB	1.92	0.99
1:A:303:GLU:OE1	1:A:340:SER:OG	1.78	0.99
1:A:519:ARG:HG2	1:A:519:ARG:HH21	1.29	0.95
1:A:337:LEU:HD12	1:A:337:LEU:C	1.82	0.95
1:A:492:HIS:HD2	1:A:494:GLU:H	1.13	0.92
1:A:519:ARG:HH21	1:A:519:ARG:CG	1.82	0.91
1:A:621:THR:HG22	1:A:624:GLU:H	1.33	0.91
1:A:546:LEU:O	1:A:546:LEU:HD23	1.70	0.91
1:A:463:ARG:HH21	1:A:463:ARG:HG2	1.35	0.91
1:A:511:LEU:HD22	1:A:515:PHE:CE2	2.06	0.91
1:A:423:GLN:HB2	1:A:425:ARG:HG3	1.53	0.90
1:A:328:GLY:O	1:A:470:ARG:NH2	2.05	0.89
1:A:307:TYR:O	1:A:310:THR:CG2	2.20	0.88
1:A:316:ARG:HB2	1:A:322:PHE:HD1	1.36	0.87
1:A:610:ILE:HG12	1:A:610:ILE:O	1.74	0.86
1:A:299:GLN:HE22	1:A:344:ALA:HB1	1.41	0.86
1:A:372:SER:O	1:A:376:VAL:HG23	1.75	0.86
1:A:266:SER:O	1:A:328:GLY:N	2.12	0.83
1:A:511:LEU:HD22	1:A:515:PHE:HE2	1.40	0.81
1:A:502:SER:HA	1:A:505:LEU:HD12	1.61	0.81
1:A:514:VAL:HG12	1:A:518:LEU:CD1	2.10	0.81
1:A:514:VAL:O	1:A:518:LEU:CD1	2.30	0.80
1:A:341:LEU:HD12	1:A:341:LEU:C	1.93	0.80
1:A:433:VAL:HG12	1:A:443:LEU:HD12	1.61	0.80
1:A:546:LEU:O	1:A:546:LEU:CD2	2.30	0.80
1:A:533:GLY:HA3	1:A:535:GLU:OE1	1.81	0.79
1:A:519:ARG:CB	1:A:519:ARG:NH2	2.46	0.79
1:A:316:ARG:HB2	1:A:322:PHE:CE1	2.17	0.79
1:A:591:ASP:HA	1:A:627:VAL:HG21	1.64	0.79
1:A:265:SER:O	1:A:367:PHE:CE2	2.35	0.78
1:A:492:HIS:HD2	1:A:494:GLU:N	1.82	0.76
1:A:546:LEU:CD2	1:A:546:LEU:C	2.54	0.76
1:A:417:LEU:HD22	1:A:468:LEU:CD2	2.13	0.75
1:A:424:ARG:O	1:A:424:ARG:HD3	1.85	0.75
1:A:225:GLN:HE22	1:A:228:ARG:HH11	1.31	0.75
1:A:578:ALA:O	1:A:613:PRO:HG2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ALA:HB2	1:A:364:LEU:HD13	1.69	0.74
1:A:250:PHE:HB2	1:A:315:THR:HG21	1.69	0.74
1:A:225:GLN:HE22	1:A:228:ARG:NH1	1.85	0.73
1:A:540:GLN:HB3	1:A:571:ASN:ND2	2.04	0.73
1:A:463:ARG:HH21	1:A:463:ARG:CG	2.02	0.72
1:A:610:ILE:HD13	1:A:612:LEU:HB2	1.71	0.71
1:A:511:LEU:CD2	1:A:515:PHE:CE2	2.72	0.71
1:A:514:VAL:HG12	1:A:518:LEU:HD11	1.73	0.70
1:A:334:ALA:HB1	1:A:364:LEU:HD22	1.72	0.70
1:A:610:ILE:CD1	1:A:612:LEU:HB2	2.21	0.70
1:A:284:LEU:HD21	1:A:288:ARG:NE	2.07	0.69
1:A:299:GLN:NE2	1:A:344:ALA:HB1	2.06	0.69
1:A:330:THR:OG1	1:A:333:GLU:CB	2.40	0.69
1:A:316:ARG:HD2	1:A:322:PHE:CE1	2.28	0.69
1:A:330:THR:OG1	1:A:333:GLU:HG2	1.89	0.69
1:A:254:LEU:HG	1:A:373:PRO:HB3	1.72	0.69
1:A:407:GLY:HA2	1:A:410:HIS:N	2.07	0.69
1:A:621:THR:HB	1:A:624:GLU:OE2	1.93	0.69
1:A:241:LEU:O	1:A:294:LYS:HE3	1.93	0.69
1:A:519:ARG:CG	1:A:519:ARG:NH2	2.47	0.69
1:A:316:ARG:HD2	1:A:322:PHE:HE1	1.57	0.68
1:A:341:LEU:HD11	1:A:345:LEU:HG	1.74	0.68
1:A:354:THR:HG21	1:A:359:VAL:HG13	1.74	0.68
1:A:639:GLN:OE1	1:A:643:GLU:HG2	1.93	0.68
1:A:485:VAL:HG21	1:A:498:LEU:HD13	1.75	0.68
1:A:452:LEU:HD22	1:A:456:GLY:HA2	1.73	0.68
1:A:488:GLN:NE2	1:A:492:HIS:HE1	1.91	0.68
1:A:492:HIS:CD2	1:A:494:GLU:H	2.04	0.68
1:A:519:ARG:HB2	1:A:519:ARG:CZ	2.23	0.68
1:A:461:ALA:O	1:A:465:LEU:HB2	1.94	0.67
1:A:593:GLU:OE2	1:A:596:LYS:HE3	1.94	0.66
1:A:489:MET:HG2	1:A:496:LEU:HD12	1.75	0.66
1:A:460:PRO:HD2	1:A:463:ARG:HD3	1.76	0.66
1:A:308:PRO:O	1:A:311:GLN:HB3	1.95	0.66
1:A:265:SER:O	1:A:367:PHE:HE2	1.78	0.65
1:A:292:LEU:O	1:A:295:ALA:HB3	1.96	0.65
1:A:259:SER:HB2	1:A:618:ARG:NH1	2.11	0.65
1:A:437:GLN:HG2	1:A:438:ASP:N	2.11	0.64
1:A:515:PHE:HA	1:A:518:LEU:HD13	1.80	0.64
1:A:640:LEU:HB3	1:A:641:PHE:CE2	2.33	0.64
1:A:284:LEU:HD21	1:A:288:ARG:CZ	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:OE2	1:A:309:GLU:N	2.30	0.63
1:A:479:ARG:NH2	1:A:513:LYS:HG3	2.14	0.63
1:A:479:ARG:CZ	1:A:513:LYS:HZ2	2.11	0.63
1:A:338:ALA:HB2	1:A:364:LEU:CD1	2.29	0.63
1:A:619:VAL:HG21	1:A:636:VAL:HG12	1.81	0.63
1:A:546:LEU:HD23	1:A:546:LEU:C	2.16	0.62
1:A:407:GLY:N	1:A:410:HIS:HB2	2.14	0.62
1:A:341:LEU:CD1	1:A:345:LEU:HG	2.30	0.62
1:A:519:ARG:CB	1:A:519:ARG:CZ	2.77	0.62
1:A:307:TYR:HB2	1:A:310:THR:CG2	2.30	0.62
1:A:591:ASP:CA	1:A:627:VAL:HG21	2.30	0.62
1:A:274:VAL:HG23	1:A:320:GLY:O	2.00	0.61
1:A:559:LEU:HD13	1:A:577:LEU:HD13	1.82	0.61
1:A:268:TYR:CZ	1:A:366:PRO:HB3	2.36	0.61
1:A:307:TYR:HB2	1:A:310:THR:HG21	1.81	0.61
1:A:248:ARG:O	1:A:252:MET:HG3	2.00	0.61
1:A:272:LEU:HD23	1:A:272:LEU:C	2.20	0.61
1:A:525:GLY:HA2	1:A:555:PHE:CD1	2.36	0.61
1:A:569:ILE:O	1:A:571:ASN:N	2.34	0.61
1:A:265:SER:HB3	1:A:369:HIS:HA	1.84	0.60
1:A:569:ILE:HG21	1:A:572:LEU:HB2	1.81	0.60
1:A:461:ALA:HB1	1:A:465:LEU:HD12	1.82	0.60
1:A:259:SER:HB2	1:A:618:ARG:CZ	2.32	0.60
1:A:250:PHE:CD1	1:A:315:THR:HG21	2.37	0.59
1:A:514:VAL:CG1	1:A:518:LEU:HD11	2.32	0.59
1:A:368:ALA:O	1:A:371:ASP:HB2	2.03	0.58
1:A:535:GLU:CD	1:A:535:GLU:H	2.06	0.58
1:A:646:PRO:O	1:A:647:TRP:C	2.41	0.58
1:A:621:THR:HG22	1:A:624:GLU:N	2.11	0.58
1:A:419:GLN:O	1:A:423:GLN:HG3	2.04	0.57
1:A:424:ARG:HG3	1:A:484:ARG:HE	1.70	0.57
1:A:424:ARG:HE	1:A:484:ARG:CG	2.16	0.57
1:A:488:GLN:NE2	1:A:492:HIS:CE1	2.72	0.57
1:A:241:LEU:H	1:A:241:LEU:CD2	2.17	0.57
1:A:253:GLN:OE1	1:A:253:GLN:HA	2.03	0.57
1:A:382:GLN:HB2	1:A:398:LEU:HD11	1.87	0.57
1:A:558:SER:HB3	1:A:579:TYR:O	2.05	0.56
1:A:267:GLY:HA2	1:A:329:MET:H	1.71	0.56
1:A:386:GLN:O	1:A:390:GLN:HG3	2.06	0.56
1:A:610:ILE:O	1:A:610:ILE:CG1	2.49	0.56
1:A:281:ASN:O	1:A:285:GLY:HA2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:OG1	1:A:333:GLU:HB2	2.05	0.55
1:A:519:ARG:HH21	1:A:519:ARG:CB	2.13	0.55
1:A:481:MET:O	1:A:485:VAL:HG23	2.06	0.55
1:A:587:ILE:HG12	1:A:616:ALA:HB1	1.89	0.55
1:A:543:LEU:O	1:A:547:THR:HG22	2.06	0.55
1:A:268:TYR:CE2	1:A:331:ARG:HA	2.42	0.55
1:A:628:ILE:HA	1:A:631:MET:HE2	1.88	0.54
1:A:546:LEU:CD2	1:A:550:LEU:HG	2.38	0.54
1:A:627:VAL:O	1:A:631:MET:HE2	2.08	0.54
1:A:519:ARG:NH2	1:A:519:ARG:HB3	2.20	0.54
1:A:489:MET:CG	1:A:496:LEU:HD12	2.37	0.54
1:A:500:LEU:HD22	1:A:530:LEU:HD13	1.89	0.54
1:A:546:LEU:C	1:A:546:LEU:HD22	2.28	0.54
1:A:414:HIS:CD2	1:A:473:TRP:CH2	2.96	0.53
1:A:225:GLN:NE2	1:A:228:ARG:HH11	2.04	0.53
1:A:511:LEU:CD2	1:A:515:PHE:HE2	2.15	0.53
1:A:512:ASN:HA	1:A:515:PHE:HD2	1.73	0.53
1:A:378:SER:O	1:A:382:GLN:HG3	2.08	0.53
1:A:293:LEU:HD23	1:A:293:LEU:N	2.23	0.53
1:A:621:THR:HG23	1:A:623:GLY:H	1.74	0.53
1:A:264:ALA:CB	1:A:265:SER:CB	2.77	0.52
1:A:407:GLY:HA2	1:A:410:HIS:H	1.73	0.52
1:A:264:ALA:CB	1:A:265:SER:HB2	2.12	0.52
1:A:424:ARG:HG2	1:A:480:LEU:HD11	1.91	0.52
1:A:424:ARG:HG3	1:A:484:ARG:HH21	1.74	0.52
1:A:269:LEU:HD12	1:A:324:VAL:O	2.10	0.52
1:A:269:LEU:O	1:A:364:LEU:HA	2.09	0.52
1:A:469:GLU:HA	1:A:469:GLU:OE1	2.10	0.52
1:A:489:MET:HG2	1:A:496:LEU:CD1	2.39	0.52
1:A:325:LEU:O	1:A:327:PRO:HD3	2.09	0.52
1:A:559:LEU:HD13	1:A:577:LEU:CD1	2.40	0.52
1:A:583:ASP:OD1	1:A:585:SER:HB3	2.09	0.52
1:A:488:GLN:HE21	1:A:492:HIS:HE1	1.58	0.51
1:A:248:ARG:HH12	1:A:596:LYS:HE3	1.75	0.51
1:A:241:LEU:H	1:A:241:LEU:HD22	1.74	0.51
1:A:627:VAL:O	1:A:627:VAL:HG12	2.11	0.51
1:A:558:SER:OG	1:A:578:ALA:HB3	2.11	0.51
1:A:577:LEU:HB2	1:A:612:LEU:HD11	1.93	0.51
1:A:270:LEU:O	1:A:323:ALA:HA	2.11	0.51
1:A:492:HIS:CD2	1:A:494:GLU:HB2	2.46	0.51
1:A:308:PRO:N	1:A:309:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:GLN:HA	1:A:614:LEU:HD22	1.92	0.51
1:A:234:THR:HA	1:A:238:GLN:HB2	1.94	0.50
1:A:620:GLU:O	1:A:640:LEU:HD13	2.11	0.50
1:A:316:ARG:HH21	1:A:319:GLY:HA2	1.77	0.50
1:A:241:LEU:HD22	1:A:241:LEU:N	2.27	0.49
1:A:284:LEU:HD22	1:A:288:ARG:HB3	1.94	0.49
1:A:386:GLN:HG2	1:A:396:ALA:CB	2.42	0.49
1:A:525:GLY:HA2	1:A:555:PHE:CE1	2.47	0.49
1:A:247:ARG:HB2	1:A:317:ILE:HG23	1.94	0.49
1:A:369:HIS:ND1	1:A:369:HIS:C	2.66	0.49
1:A:362:ILE:O	1:A:395:TRP:HA	2.13	0.49
1:A:523:ASN:OD1	1:A:523:ASN:O	2.30	0.49
1:A:540:GLN:CD	1:A:569:ILE:O	2.51	0.48
1:A:386:GLN:HG2	1:A:396:ALA:HB1	1.95	0.48
1:A:434:VAL:HG22	1:A:636:VAL:HG23	1.95	0.48
1:A:311:GLN:O	1:A:312:ASN:HB2	2.11	0.48
1:A:318:ARG:O	1:A:319:GLY:C	2.50	0.48
1:A:460:PRO:O	1:A:462:GLY:N	2.46	0.48
1:A:485:VAL:O	1:A:489:MET:HG3	2.13	0.48
1:A:582:ILE:HG22	1:A:583:ASP:O	2.14	0.48
1:A:335:LEU:O	1:A:339:GLN:HG3	2.14	0.48
1:A:424:ARG:O	1:A:424:ARG:CD	2.57	0.48
1:A:544:GLU:O	1:A:548:ARG:HG2	2.14	0.48
1:A:316:ARG:CB	1:A:322:PHE:HD1	2.18	0.48
1:A:342:ASP:HB2	1:A:362:ILE:HD13	1.94	0.48
1:A:448:LEU:HD23	1:A:644:PRO:HB3	1.95	0.48
1:A:248:ARG:NH1	1:A:596:LYS:HE3	2.28	0.48
1:A:254:LEU:CG	1:A:373:PRO:HB3	2.42	0.48
1:A:268:TYR:HE2	1:A:331:ARG:HA	1.79	0.48
1:A:426:PHE:CD1	1:A:451:LEU:HA	2.49	0.48
1:A:548:ARG:HG3	1:A:549:ARG:N	2.29	0.48
1:A:492:HIS:CD2	1:A:494:GLU:N	2.70	0.47
1:A:548:ARG:HG3	1:A:549:ARG:H	1.79	0.47
1:A:272:LEU:HD11	1:A:345:LEU:HD11	1.97	0.47
1:A:272:LEU:HD22	1:A:322:PHE:HD2	1.79	0.47
1:A:365:ALA:HB2	1:A:380:GLY:HA2	1.96	0.47
1:A:641:PHE:CD2	1:A:641:PHE:N	2.83	0.47
1:A:504:THR:O	1:A:511:LEU:HB2	2.15	0.47
1:A:512:ASN:O	1:A:513:LYS:C	2.53	0.47
1:A:537:LEU:HD22	1:A:543:LEU:HD22	1.97	0.47
1:A:619:VAL:HG21	1:A:636:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TYR:HE1	1:A:333:GLU:OE1	1.98	0.47
1:A:514:VAL:CG1	1:A:518:LEU:CD1	2.86	0.47
1:A:591:ASP:HB3	1:A:627:VAL:CG2	2.45	0.47
1:A:424:ARG:CG	1:A:484:ARG:HE	2.28	0.46
1:A:389:GLY:O	1:A:390:GLN:HG2	2.15	0.46
1:A:272:LEU:O	1:A:321:GLU:HA	2.16	0.46
1:A:621:THR:CG2	1:A:624:GLU:H	2.17	0.46
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.58	0.46
1:A:640:LEU:HD23	1:A:641:PHE:CZ	2.50	0.46
1:A:463:ARG:CG	1:A:463:ARG:NH2	2.70	0.46
1:A:253:GLN:O	1:A:257:ARG:HB2	2.14	0.46
1:A:625:LEU:O	1:A:625:LEU:HD12	2.16	0.46
1:A:265:SER:N	1:A:369:HIS:HB2	2.31	0.46
1:A:591:ASP:HB3	1:A:627:VAL:HG21	1.97	0.46
1:A:275:LYS:HD2	1:A:358:ALA:HB3	1.98	0.45
1:A:287:GLN:HE21	1:A:287:GLN:HB3	1.61	0.45
1:A:399:ASP:N	1:A:399:ASP:OD2	2.47	0.45
1:A:546:LEU:O	1:A:546:LEU:HD22	2.13	0.45
1:A:610:ILE:HD13	1:A:612:LEU:CB	2.42	0.45
1:A:307:TYR:C	1:A:309:GLU:OE2	2.54	0.45
1:A:386:GLN:HG3	1:A:390:GLN:HE21	1.81	0.45
1:A:590:ILE:HD13	1:A:631:MET:HE1	1.99	0.45
1:A:569:ILE:CG2	1:A:572:LEU:HB2	2.46	0.45
1:A:330:THR:HG1	1:A:333:GLU:CG	1.90	0.45
1:A:460:PRO:O	1:A:461:ALA:C	2.53	0.45
1:A:539:GLU:C	1:A:541:ALA:N	2.68	0.45
1:A:542:VAL:O	1:A:545:GLN:HB2	2.17	0.45
1:A:494:GLU:O	1:A:527:ARG:NE	2.47	0.45
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.84	0.45
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.66	0.45
1:A:417:LEU:CD2	1:A:468:LEU:HD21	2.25	0.45
1:A:540:GLN:NE2	1:A:569:ILE:C	2.71	0.45
1:A:544:GLU:OE2	1:A:571:ASN:ND2	2.44	0.45
1:A:571:ASN:O	1:A:575:LEU:HG	2.17	0.45
1:A:234:THR:HA	1:A:238:GLN:CB	2.48	0.44
1:A:254:LEU:CD2	1:A:373:PRO:HB3	2.47	0.44
1:A:590:ILE:HG23	1:A:627:VAL:HG11	1.99	0.44
1:A:453:ASP:O	1:A:454:GLU:C	2.55	0.44
1:A:484:ARG:HA	1:A:484:ARG:HD2	1.79	0.44
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.74	0.44
1:A:259:SER:HB2	1:A:618:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.64	0.44
1:A:307:TYR:CD1	1:A:329:MET:CE	3.00	0.44
1:A:511:LEU:CD2	1:A:511:LEU:O	2.66	0.44
1:A:283:ARG:NH2	1:A:283:ARG:HB2	2.33	0.44
1:A:346:SER:HA	1:A:359:VAL:HG21	1.99	0.44
1:A:582:ILE:O	1:A:583:ASP:C	2.56	0.43
1:A:284:LEU:HD11	1:A:288:ARG:HE	1.83	0.43
1:A:339:GLN:O	1:A:343:SER:OG	2.30	0.43
1:A:507:ASP:OD1	1:A:509:GLN:HB3	2.18	0.43
1:A:511:LEU:CD2	1:A:511:LEU:C	2.86	0.43
1:A:478:ASP:OD2	1:A:501:SER:HB3	2.18	0.43
1:A:250:PHE:CD1	1:A:315:THR:CG2	3.01	0.43
1:A:241:LEU:CD2	1:A:241:LEU:N	2.82	0.43
1:A:358:ALA:O	1:A:360:ALA:N	2.52	0.43
1:A:591:ASP:CB	1:A:627:VAL:HG21	2.49	0.43
1:A:281:ASN:O	1:A:285:GLY:CA	2.67	0.43
1:A:484:ARG:N	1:A:484:ARG:CD	2.81	0.43
1:A:316:ARG:O	1:A:316:ARG:HG2	2.18	0.42
1:A:296:VAL:O	1:A:297:GLY:C	2.56	0.42
1:A:424:ARG:HE	1:A:484:ARG:HG3	1.84	0.42
1:A:260:ASN:HA	1:A:261:PRO:HD2	1.67	0.42
1:A:264:ALA:HA	1:A:265:SER:HA	1.75	0.42
1:A:331:ARG:CG	1:A:332:GLU:N	2.82	0.42
1:A:513:LYS:HA	1:A:513:LYS:HD2	1.66	0.42
1:A:252:MET:HE3	1:A:596:LYS:HE2	2.00	0.42
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.62	0.42
1:A:276:ASP:O	1:A:280:LEU:HD22	2.20	0.42
1:A:414:HIS:HA	1:A:471:PHE:CE2	2.55	0.42
1:A:311:GLN:O	1:A:312:ASN:CB	2.68	0.41
1:A:276:ASP:OD2	1:A:283:ARG:NH1	2.52	0.41
1:A:599:PHE:CZ	1:A:603:ILE:HD11	2.54	0.41
1:A:247:ARG:HE	1:A:247:ARG:HB3	1.05	0.41
1:A:284:LEU:HD13	1:A:288:ARG:HG2	2.02	0.41
1:A:459:ILE:HA	1:A:460:PRO:HD3	1.87	0.41
1:A:540:GLN:HB3	1:A:571:ASN:HD21	1.80	0.41
1:A:250:PHE:HD1	1:A:315:THR:HG21	1.82	0.41
1:A:389:GLY:O	1:A:390:GLN:CG	2.68	0.41
1:A:464:PHE:CD1	1:A:464:PHE:C	2.94	0.41
1:A:507:ASP:O	1:A:511:LEU:HB2	2.21	0.41
1:A:408:ASP:HA	1:A:409:ASP:HA	1.47	0.41
1:A:537:LEU:HD22	1:A:543:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:VAL:O	1:A:627:VAL:CG1	2.68	0.40
1:A:232:LEU:HD12	1:A:232:LEU:O	2.21	0.40
1:A:480:LEU:O	1:A:480:LEU:HD12	2.21	0.40
1:A:513:LYS:C	1:A:513:LYS:HE2	2.41	0.40
1:A:569:ILE:O	1:A:571:ASN:OD1	2.38	0.40
1:A:450:ARG:HD3	1:A:450:ARG:HA	1.84	0.40
1:A:550:LEU:HD22	1:A:550:LEU:HA	1.80	0.40
1:A:612:LEU:HA	1:A:613:PRO:HD2	1.76	0.40
1:A:424:ARG:HH11	1:A:484:ARG:CG	2.35	0.40
1:A:502:SER:O	1:A:506:ALA:N	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	419/430 (97%)	377 (90%)	39 (9%)	3 (1%)	22 57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	GLY
1	A	359	VAL
1	A	647	TRP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	342/348 (98%)	263 (77%)	79 (23%)	1 3

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	A	229	SER
1	A	231	LYS
1	A	241	LEU
1	A	247	ARG
1	A	257	ARG
1	A	259	SER
1	A	262	GLU
1	A	265	SER
1	A	266	SER
1	A	268	TYR
1	A	273	ARG
1	A	277	LEU
1	A	280	LEU
1	A	281	ASN
1	A	282	GLN
1	A	284	LEU
1	A	287	GLN
1	A	288	ARG
1	A	293	LEU
1	A	302	ARG
1	A	309	GLU
1	A	310	THR
1	A	311	GLN
1	A	312	ASN
1	A	315	THR
1	A	316	ARG
1	A	318	ARG
1	A	325	LEU
1	A	331	ARG
1	A	336	GLN
1	A	337	LEU
1	A	340	SER
1	A	341	LEU
1	A	359	VAL
1	A	364	LEU

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Mol	Chain	Res	Type
1	A	369	HIS
1	A	372	SER
1	A	386	GLN
1	A	397	CYS
1	A	408	ASP
1	A	417	LEU
1	A	419	GLN
1	A	424	ARG
1	A	437	GLN
1	A	439	THR
1	A	441	LEU
1	A	443	LEU
1	A	448	LEU
1	A	454	GLU
1	A	457	GLN
1	A	463	ARG
1	A	465	LEU
1	A	479	ARG
1	A	484	ARG
1	A	488	GLN
1	A	504	THR
1	A	505	LEU
1	A	509	GLN
1	A	511	LEU
1	A	513	LYS
1	A	516	GLU
1	A	519	ARG
1	A	522	SER
1	A	532	ILE
1	A	539	GLU
1	A	544	GLU
1	A	546	LEU
1	A	550	LEU
1	A	551	ARG
1	A	556	SER
1	A	565	ARG
1	A	598	LEU
1	A	610	ILE
1	A	621	THR
1	A	628	ILE
1	A	636	VAL
1	A	641	PHE

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Mol	Chain	Res	Type
1	A	647	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	225	GLN
1	A	287	GLN
1	A	336	GLN
1	A	393	GLN
1	A	419	GLN
1	A	444	HIS
1	A	488	GLN
1	A	492	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	423/430 (98%)	-0.17	0	100	100	44, 83, 125, 185	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.